# Estimating and controlling numerical error in simulations using spatial

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Brian Carnes
bcarnes@sandia.gov
Nick Alger
nalger@ices.utexas.edu

Sandia National Laboratories
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- Overview of random fields and non-intrusive UQ
- Some verification test problems (1D/2D)
- Error estimation for KL eigenproblem
- Error estimation for KL random fields
- Adaptivity demonstration

# Overview

- General stochastic fields in space/time can be modeled as random fields (RFs) / stochastic processes
- The most efficient representation of RFs are KL series
- Polynomial Chaos (PC) expansions are also popular
- Non-intrusive uncertainty quantification (UQ) is a technique for embedding deterministic solvers in a UQ loop
- Each realization of a RF in a non-intrusive UQ algorithm determines a heterogeneous field
- Our goal: quantify and reduce the (deterministic) error in RF realizations
- Longer term we plan to work on adaptive methods to equilibrate all sources of error

# Non-intrusive UQ with Random Fields

- RF Simulator added to traditional non-intrusive UQ coupling
- RV coeffs $\{\xi_j\}$ are now DoFs for random field $\alpha(x, \xi)$, such as through a Karhunen-Loeve (KL) series

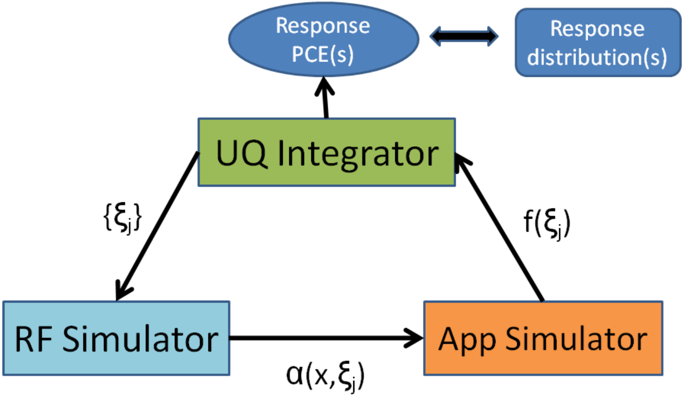



Figure: Overview of non-intrusive UQ coupled multiphysics.

# Overview: KL Series Representation

- A random field $\alpha(x, \omega)$ assigns a *random variable* (RV) to each point $x \in D$.
- RFs are defined on the product space of $L^2(D)$ and $L^2_{\mathcal{P}}(\Omega)$, where $(\Omega, \mathcal{S}, \mathcal{P})$ is a probability space.
- The Karhunen-Loeve expansion of a (separable, second order) random field takes the form

$$\alpha(x, \omega) = m(x) + \sum_{j=1}^{\infty} \xi_j(\omega) \sqrt{\lambda_j}\, \phi_j(x) \tag{1}$$

- Data required: mean $m(x) = E[\alpha(x)]$ and covariance function

$$r(x, y) \equiv E[(\alpha(x) - m)\,(\alpha(y) - m)]$$

- The covariance function can be parametric (assumed functional form) or can be determined from experimental data.

# Overview: KL Eigenvalue Problem

- The KL eigenproblem: find $\{\phi_j, \lambda_j\} \in L^2(D) \times \mathbb{R}$:

$$
\begin{aligned}
B(\phi_j, v) &= \lambda_j (\phi_j, v)_D, \quad v \in L^2(D), \\
B(w, v) &\equiv \int_D \int_D r(x,y)\, w(y)\, v(x)\, dy\, dx \\
(\phi_i, \phi_j)_D &= \delta_{ij}
\end{aligned}
$$

- The uncorrelated RV coefficients $\xi_j$ are defined by

$$
\begin{aligned}
\xi_j &\equiv \frac{1}{\sqrt{\lambda_j}} \int_D (\alpha(x) - m)\, \phi_j(x)\, dx \\
E[\xi_i\, \xi_j] &= \delta_{ij}
\end{aligned}
$$

# Approximation of the KL Eigenproblem

- We consider Galerkin finite element approximations using subspaces $V_h \subset L^2(D)$
- Piecewise discontinuous (or continuous) polynomials of order $p \geq 0$ are used.
- The discrete KL eigenproblem: find $\{\phi_{j,h}, \lambda_{j,h}\} \in V_h \times \mathbb{R}$:

$$
\begin{aligned}
B(\phi_{j,h}, v_h) &= \lambda_{j,h}(\phi_{j,h}, v_h), \quad v_h \in V_h, \\
\|\phi_{j,h}\| &= 1
\end{aligned}
$$

- The matrix for the approximated bilinear form is a dense matrix.

# Verification Test Problem (1D)

- We used a 1D problem on $D = (-1, 1)$ with $r(x, y) \equiv \exp(-|x - y|)$.
- The exact KL eigensolution can be computed (Ghanem and Spanos, 1991).
- The RV coefficients $\xi_j$ are independent standard Gaussians.

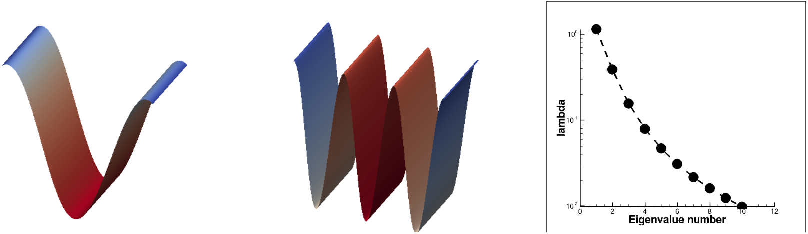
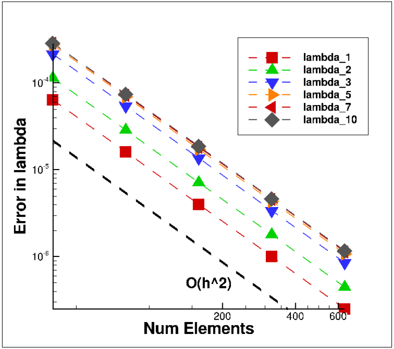



Figure: Eigenfunctions 3 and 7. First 10 eigenvalues

# Verification Of Convergence (1D)

- Approximate a priori convergence rates are

$$|\lambda - \lambda_h| \approx \lambda^{-1/2}\, h^{2(p+1)}, \quad \|\phi - \phi_h\| \approx \lambda^{-3/2}\, h^{p+1}$$



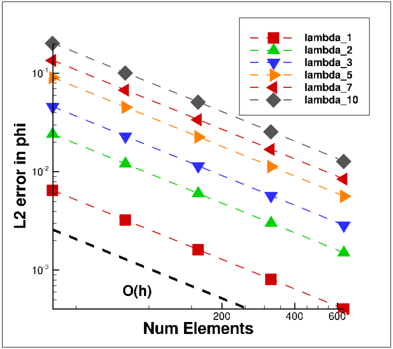




Figure: Lowest order case ($p = 0$): (left) error in $\lambda$, (right) error in $\phi$

# Verification Test Problems (2D)

- Tensor product covariance function

$$r(\mathbf{x},\mathbf{y}) = \prod_{i=1}^{dim} \exp(-|x_i - y_i|/L_i)$$

  allows KL solution on rectangle based on products of 1D solutions.
- Case 1: $D = (-1,1)^2$ and $L_1 = L_2 = 1$. Here we get pairs of repeated eigenvalues.
- Case 2: $D = (-1,1)$, $L_1 = 1$ and $L_2 = 2/3$. Here we get only unique eigenvalues (although they cluster as $i \gg 1$).

# Verification Of Convergence (2D)

- We report convergence rates similar to the 1D results for the case of unique eigenvalues.

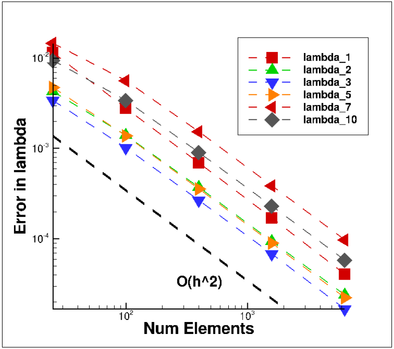



Figure: Unique eigenvalue case: error in $\lambda$

# A Posteriori Error Estimation for KL Eigenproblem

- The residual (for a given eigenpair) is

$$R \equiv R(\phi_h, \lambda_h) \equiv -K\,\phi_h + \lambda_h\,\phi_h$$

- Defining errors $e \equiv \phi - \phi_h$ and $\mu \equiv \lambda - \lambda_h$, we have the residual-error relation:

$$R = K\,e - \lambda\,e - \mu\,\phi_h$$

- Larson's approach (SINUM, '00) defines auxiliary functions $z$ so that $(R, z)$ approximates either $\mu$ or $\|e\|^2$.
- We use a simpler approach based on choosing either $z = \phi$ or $z = e$.

# Error Estimates for $\mu$

- Here we multiple by $\phi$ and integrate to derive

$$(R, \phi) = \mu \, (1 - \frac{1}{2} \|e\|^2)$$

- Applying error orthogonality, Cauchy-Schwartz and interpolation estimates, we have

$$|(R, \phi)| \leq C \|h^{p+1} \, R\| |\phi|_{p+1}$$

- We can estimate $D^\alpha \phi$ for any $|\alpha| = p + 1$ using the integral equation

$$\begin{aligned} D_x^\alpha \phi(x) &= \frac{1}{\lambda} \int_D D_x^\alpha r(x, y) \, \phi(y) \, dy \\ |\phi|_{p+1} &\leq \frac{1}{\lambda} |r|_{p+1,x} \end{aligned}$$

# Error Estimates for $\mu$ (2)

- Combining the estimates we have

$$\mu\,(1 - \frac{1}{2}\|e\|^2) \le C\,\lambda^{-1}\,\|h^{p+1}\,R\|\,|r|_{p+1,x}$$

- It was assumed in Larson that $\|e\|^2$ is small enough to be absorbed into the constant.
- In practice we see that

$$\mu \approx C\,\lambda^{-1/2}\,\|h^{p+1}\,R\|$$

which suggests that the factor $\lambda^{-1}$ increases to $\lambda^{-1/2}$ through the term $(1 - \frac{1}{2}\|e\|^2)$.

# Error Estimates for $\|e\|$

- Here we multiple by $e$ and integrate to derive

$$(R,e) = (K\,e,e) - \lambda\|e\|^2 - \mu\,(\phi_h,e)$$

- We have $-(\phi_h,e) = \frac{1}{2}\,\|e\|^2$ and can estimate

$$\frac{\lambda}{2}\,\|e\|^2 \le (K\,e,e) \le \frac{\lambda+\lambda_{max}}{2}\,\|e\|^2$$

- We obtain the upper bound on $\|e\|$

$$\|e\| \le \frac{1}{\lambda}\,\|R\|$$

# Effectiveness of KL Error Estimators (1D)

- We test the KL error indicators using the 1D verification test.
- The estimate for $\mu$ overestimates by about 3-6; however both scale well with $h$ and $\lambda$

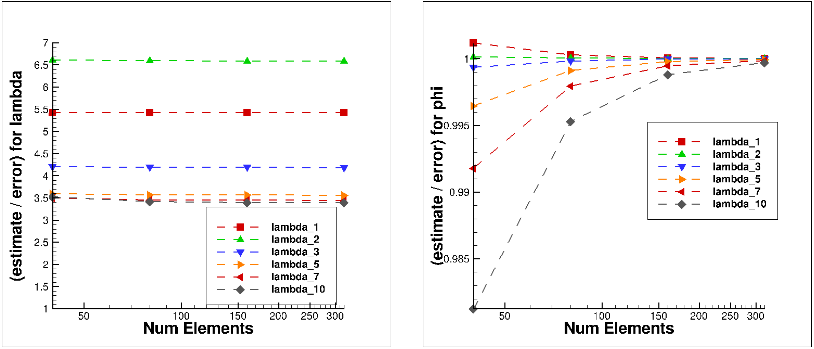



Figure: (left) indicator/error ratio for $\lambda$, (right) indicator/error ratio for $\phi$

# A Posteriori Error Estimation for KL Realizations

- For non-intrusive UQ, we are given a realization of the RVs.
- Consider an $N$ term truncated KL series with fixed RV weights $\{\xi_i\}$.
- The truncated KL series is approximated as

$$\alpha(x) = \sum_{i=1}^{N} \xi_i \sqrt{\lambda_i}\, \phi_i(x) \approx \alpha_h(x) \equiv \sum_{i=1}^{N} \xi_i \sqrt{\lambda_{i,h}}\, \phi_{i,h}(x)$$

- The error estimation problem is then deterministic.
- Our interest is in estimating $\|e_\alpha\| \equiv \|\alpha - \alpha_h\|$

# Error in Truncated KL Series

- The error can be linearized as:

$$\|e_\alpha\| \approx E \equiv \left\| \sum_{i=1}^{N} \xi_i \left( \frac{1}{2\sqrt{\lambda_{i,h}}} \mu_i \, \phi_{i,h} + \sqrt{\lambda_{i,h}} \, e_i \right) \right\|$$

- The simplest estimate is to use the triangle inequality:

$$E \leq \sum_{i=1}^{N} |\xi_i| \left( \frac{1}{2\sqrt{\lambda_{i,h}}} |\mu_i| + \sqrt{\lambda_{i,h}} \, \|e_i\| \right)$$

- Bounding $\mu_i$ and $\|e_i\|$ by our previous estimates, we obtain our first estimator, denoted $\eta^{TI}$

# Error in Truncated KL Series (2)

- Expanding $E^2$ into $4\,N^2$ terms, we can develop more refined estimates.

$$
\begin{aligned}
E^2 &= \sum_{i,j}^{N} \xi_i\, \xi_j \Big( \frac{1}{2\sqrt{\lambda_{i,h}}}\, \mu_i\, \phi_{i,h} + \sqrt{\lambda_{i,h}}\, e_i, \frac{1}{2\sqrt{\lambda_{j,h}}}\, \mu_j\, \phi_{j,h} + \sqrt{\lambda_{j,h}}\, e_j \Big) \\
&= \sum_{i}^{N} \xi_i^2 \{ \frac{1}{4\lambda_{i,h}}\, \mu_i^2 + \lambda_{i,h}\, \|e_i\|^2 \} \\
&+ 2 \sum_{i,j}^{N} \xi_i\, \xi_j\, \frac{\sqrt{\lambda_{j,h}}}{2\sqrt{\lambda_{i,h}}}\, \mu_i (\phi_{i,h}, e_j) \\
&+ \sum_{i,j\neq i}^{N} \xi_i\, \xi_j\, \sqrt{\lambda_{i,h}}\, \sqrt{\lambda_{j,h}} (e_i, e_j) \\
&= I + II + III
\end{aligned}
$$

# Error in Truncated KL Series (3)

- We are interested in estimators that are optimal over any number of terms $N$
- We define $\eta^{DIAG}$ using term $I$ (diagonal terms, all non-negetive) with our estimates for $\mu_i$ and $\|e_i\|$.
- Terms $II$ and $III$ contain signed terms and possible cancellations.
- Term $II$ is a higher order term.
- We define $\eta^{AT}$ using bounds on both term $I$ and $III$

$$|III| \leq (\sum_{i}^{N} \lambda_{i,h}) \sum_{j}^{N} \xi_j^2 \|e_j\|^2$$

# Effectiveness of Various RF Error Estimators (1D)

- We test the RF error estimators using the 1D verification test.
- Here we take 10 terms with $\xi_j \equiv 1$.

| Num Elems | $\eta^{TI}$ | $\eta^{DIAG}$ | $\eta^{AT}$ |
|---|---|---|---|
| 40 | 4.1764 | 1.2006 | 10.7214 |
| 80 | 3.9402 | 1.1953 | 10.8810 |
| 160 | 3.8142 | 1.1938 | 10.9213 |
| 320 | 3.7496 | 1.1934 | 10.9314 |
| 640 | 3.7169 | 1.1933 | 10.9339 |

Table: Ratio of error indicator to true error for 10 term 1D random field.

- Note that $\eta^{TI}$ and $\eta^{AT}$ overestimate the error by about $\sqrt{N}$ and $N$, respectively.

# Adaptive Mesh Refinement for RFs

- Adaptive loop for RFs:
  - run KL eigensolver and compute RF realization
  - compute RF error indicator and local indicator
  - mark and refine elements
- One problem is sign-flipping in the eigenvectors.
- This has been (partially) fixed by controlling the sign by projection on a fixed vector.

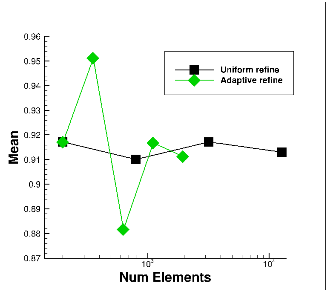
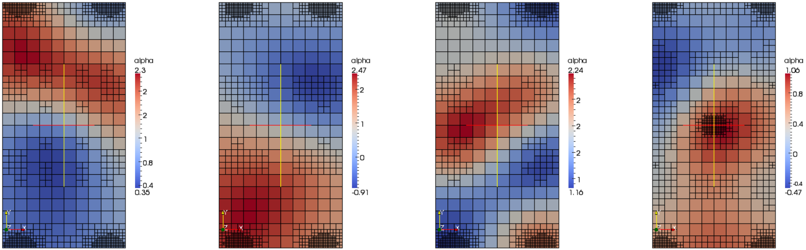



Figure: Convergence of mean under uniform and adaptive refinement.

# Examples of Adapted RF Realizations

- We generated several RF realizations using 10 KL terms and LHS sampling (from DAKOTA).
- The response function is a point value evaluation of the RF.




- LHS integration tests includes all modes (espec. high frequency)
- Sparse grid integration methods tend to use a small number of terms

# Convergence in Distribution

- We see that AMR can produce convergent distributions, here using a level one sparse grid.

| elements | $p = 0.5$ | $p = 0.9$ | $p = 0.99$ |
|---|---|---|---|
| **Adaptive refinement** | | | |
| 200 | 0.969280 | 2.15575 | 3.12044 |
| 356 | 0.997643 | 2.16958 | 3.14831 |
| 632 | 0.993912 | 2.17601 | 3.13616 |
| 1112 | 0.999326 | 2.18310 | 3.15057 |
| **Uniform refinement** | | | |
| 800 | 1.00033 | 2.18107 | 3.13828 |
| 3200 | 1.00064 | 2.18050 | 3.12973 |

# Conclusions

- Spatial error from heterogeneous random fields may be significant in UQ calculations
- A posteriori error estimation techniques can be effective in estimating RF error.
- Adaptivity based on RF error can be effective, although more efficient algorithms may be possible.
- Future work:
  - Develop goal-oriented approaches for output quantities.
  - Include other sources of error: UQ integration, KL series truncation